- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

October 1986.

CRITICAL EVALUATION:

Quantitative solubility data for the ethylbenzene (1) - water (2) system have been reported in the publications listed in Table 1.

TABLE 1: Quantitative Solubility Studies of the Ethylbenzene (1) - Water (2) System

Reference	T/K	Solubility	Method
Fühner (ref 1)	288	(1) in (2)	titration
Andrews and Keefer (ref 2)	298	(1) in (2)	spectrophotometric
Klevens (ref 3)	298	(1) in (2)	spectrophotometric
Bohon and Claussen (ref 4)	273-316	(1) in (2)	spectrophotometric
Filippov and Furman (ref 5)	291-323	(2) in (1)	synthetic
Morrison and Billett (ref 6)	298	(1) in (2)	analytical
Jones and Monk (ref 7)	298-308	(2) in (1)	radiotracer
McAuliffe (ref 8)	298	(1) in (2)	GLC
Guseva and Parnov (ref 9)	338-507 ^a	(1) in (2)	unspecified
Englin et al. (ref 10)	283-303	(2) in (1)	analytical
McAuliffe (ref 11)	298	(1) in (2)	GLC
Polak and Lu (ref 14)	273,298	mutual	GLC, Karl Fischer
Brown and Wasik (ref 15)	278-293	(1) in (2)	chromatographic
Sutton and Calder (ref 16)	298	(1) in (2)	GLC
Price (ref 17)	298	(1) in (2)	GLC
Korenman and Aref'eva (ref 18	3) 293	(1) in (2)	titration
Korenman and Aref'eva (ref 19	9) 298	(1) in (2)	titration
Krzyzanowska and Szeliga (ref 20)	298	(1) in (2)	GLC
Sanemasa et al . (ref 21,22)	288-318	(1) in (2)	spectrophotometric
Sanemasa et al . (ref 23)	298	(1) in (2)	spectrophotometric
Heidman et al. (ref 24)	311 - 568 ^a	mutual	GLC, Karl Fischer

a Pressure also varied, see Table 6.

The original data in all of these publications are compiled in the Data Sheets immediately following this Critical Evaluation. Critical phenomena at high pressures have been reported by Alwani and Schneider (ref 12) and Roof (ref 13) and are discussed along with the high pressure solubility data (ref 9, 24) in Section 3 below. For convenience, further discussion of this system will be divided into three parts.

COMPONENTS:	EVALUATOR:
(2) Water: H ₋ O: [7732-18-5]	G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	October 1986.

CRITICAL EVALUATION: (continued)

In the tables which follow values marked with an asterisk (*) have been obtained by the Evaluator by graphical interpolation of the original authors' experimental data. "Best" values have been obtained by averaging all non-rejected data. Standard deviations (σ_n) have been included as a convenient measure of the spread of experimental results: they do not have any statistical significance.

1. SOLUBILITY OF ETHYLBENZENE (1) IN WATER (2)

Of the data available on the solubility of ethylbenzene in water, values of Bohon and Claussen (ref 4) and Korenman and Aref'eva (ref 18) have been rejected because they are significantly higher (by about 10%) than all other studies. The value of Price (ref 17) at 298K is markedly lower than all other studies and is also rejected. The datum of Krzyzanowska and Szeliga (ref 20) has been excluded from consideration because it does not appear to have been obtained independently of that of Price (ref 17). The remaining data are summarized in Table 2 and are generally in excellent agreement even though few studies have covered the same temperature range (which has limited the number of Recommended values). Selected data are also plotted in Figure 1.

TABLE 2: Recommended (R) and Tentative Values of the Solubility of Ethylbenzene (1) in Water (2)

T/K	Solubility	y values	
	Reported values	"Best" values	
	10 ² g(1)/100g sln	10 ² g(1)/100g sln	$10^5 x_1$
273	1.97 (ref 14)	2.0	3.4
283	1.84* (ref 15)	1.8	3.1
293	1.84* (ref 15), 1.77 (ref 21)	$1.81 \pm 0.04 (R)$	3.07 (R)
298	1.68 (ref 2), 1.75 (ref 3), 1.65 (ref 6), 1.59 (ref 8), 1.52 (ref 11), 1.77 (ref 14), 1.61 (ref 16), 1.8 (ref 19), 1.81 (ref 21), 1.69 (ref 22), 1.72 (ref 23)	1.69 ± 0.09 (R)	2.87 (R)
303	1.86* (ref 21)	1.9	3.2
313	$2.03*$ (ref 21), 1.97^a (ref 24)	$2.00 \pm 0.03 (R)$	3.39 (R)
323	2.19 ^a (ref 24)	2.2	3.7
333	2.47^{α} (ref 24)	2.5	4.2
343	2.83 ^a (ref 24)	2.8	4.8

(Table 2 continued next page)

- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

October 1986.

CRITICAL EVALUATION: (continued)

Table 2 (continued)

T/K	Solubility	Solubility values	
	Reported values	"Best" values	
	10 ² g(1)/100g sln	10 ² g(1)/100g sln	$10^5 x_1$
353	3.28 ^a (ref 24)	3.3	5.6
363	3.86 ^a (ref 24)	3.9	6.6
373	4.60 ^a (ref 24)	4.6	7.8

a Calculated over the stated experimental range from the fitting equation given by the original authors.

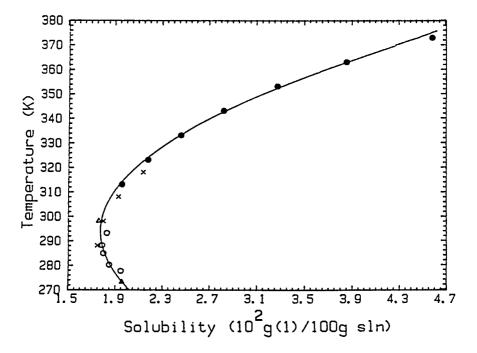


FIGURE 1: Solubility of ethylbenzene in water, selected data: ref 14 (Δ); ref 15 (o); ref 21 (x); ref 24 (\bullet). The solid curve has been fitted to the "Best" values (Table 2).

Thermodynamic functions for the dissolution of ethylbenzene in water derived by application of the van't Hoff equation are summarized in Table 3. With the exception of the data of Brown and Wasik (ref 15) which were obtained over a limited temperature range (Table 1), the $\Delta H_{\rm Sln}$ and $\Delta C_{\rm p,sln}$ derived from the various values are quite close to reliable calorimetric values reported for the dissolution of benzene in water. This gives added confidence to the solubility data in Table 2. (continued next page)

COMPONENTS: (1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4] (2) Water; H ₂ O; [7732-18-5]	EVALUATOR: G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.
	October 1986.

CRITICAL EVALUATION: (continued)

TABLE 3: Thermodynamic Functions for the Dissolution of Ethylbenzene in Water Derived from Solubility Data

Reference	^{ΔH} sln kJ mol-l	$^{\Delta C}$ p,sln . J K ⁻¹ mol ⁻¹
Brown and Wasik (ref 15)	11.9	1123
Sanemasa et al . (ref 21)	3.6	319
Sanemasa et al. (ref 22)	3.9	230
Heidman et al. (ref 24)	4.5	213
"Best" values (Table 2)	2.1	275

2. SOLUBILITY OF WATER (2) IN ETHYLBENZENE (1) With the exception of the data of Jones and Monk (ref 7) which are reported in v/v fractions, all the available values for the solubility of water in ethylbenzene are summarized in Table 4 below. Unfortunately, few of the determinations cover the same temperature range. Where comparison is possible at lower temperatures ($T \le 298$ K) independent determinations are in reasonable agreement. At higher temperatures (T > 298K) the values of

TABLE 4: Recommended (R) and Tentative Values of the Solubility of Water (2) in Ethylbenzene (1)

Filippov and Furman (ref 5) and Heidman et al. (ref 24) show an increasing

divergence with increasing temperature (Figure 2).

T/K	Solubility	values	
	Reported values	"Best" values	$(\pm \sigma_n)$
	10 ² g(2)/100g sln	10 ² g(2)/100g sln	10 ³ x ₂
273	1.78 (ref 14)	1.8	1.1
283	2.75 (ref 10)	2.8	1.7
293	3.3* (ref 5), 3.73 (ref 10)	3.5 ± 0.2	2.1
298	4.2* (ref 5), 4.4* (ref 10), 4.42 (ref 14)	4.3 ± 0.1 (R)	2.5 (R)
303	5.9* (ref 5), 5.02 (ref 10)	5.5 ± 0.5	3.2
313	9.6* (ref 5), 7.2^{a} (ref 24)	8 ± 1	5
323	13.3* (ref 5), 9.68 a (ref 24)	11 ± 2	6
333	12.9 ^a (ref 24)	13	8
343	16.9 ^a (ref 24)	17	10
353	21.9 ^a (ref 24)	22	13
363	28.0 ^a (ref 24)	28	17
373	35.6 ^a (ref 24)	36	21

a Calculated over the stated experimental range by the fitting equation given by the original authors. (continued next page)

- (1) Ethylbenzene; C_8H_{10} ; 100-41-4
- (2) Water; H₂O; 7732-18-5

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

October 1986

CRITICAL EVALUATION: (continued)

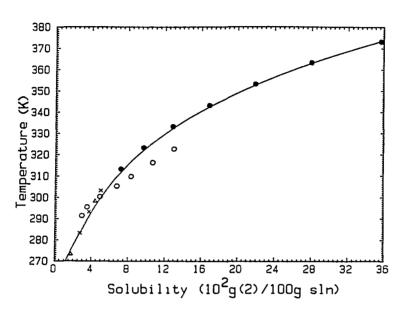


FIGURE 2. Solubility of water in ethylbenzene: ref 5 (o); ref 10 (x); ref 14 (Δ); ref 24 (\bullet). Solid line is fitted to "Best" values from Table 4.

Thermodynamic functions derived by application of the van't Hoff equation to the various data sets are summarized in Table 5.

TABLE 5: Thermodynamic functions for the Dissolution of Water in Ethylbenzene Derived from Solubility Data

Reference	ΔH _{sln} kJ mol-1	ΔCp,sln J K-1 mol-1
 Filippov and Furman (ref 5)	45.2	-809
Englin et al. (ref 10)	22.0	91
Heidman et al. (ref 24)	24.4	33

The thermodynamic functions derived from the data of both Englin $et\ al.$ (ref 10) and Heidman $et\ al.$ (ref 24) are comparable to those obtained for related, well characterized systems (e.g. water in benzene) whereas the values of Filippov and Furman (ref 5) are not. Further investigation of this system is clearly warranted.

- (1) Ethylbenzene; C_8H_{10} ; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia.

October 1986.

CRITICAL EVALUATION: (continued)

3. MUTUAL SOLUBILITIES OF ETHYLBENZENE (1) AND WATER (2) AT ELEVATED TEMPERATURES

To clarify the relationship between the phases in equilibrium it is convenient to consider the pressure-temperature projection of the pressure-temperature-composition diagram for this system. On such a diagram (Figure 3) phases with the same value of pressure and temperature but different composition will be located at the same point. The general typology of the phase diagram of this system is similar to that of benzene + water (except that the vapor pressure of ethylbenzene is considerably less than that of benzene). Ethylbenzene + water has type III phase behaviour (using Scott and von Konynenberg's classification (ref 25, 26). This type of phase behaviour is characterized by two critical loci, with one starting at the critical point of the pure component with the higher critical temperature (water in this case) and eventually approaching high pressures. The other critical locus starts at the critical point of the other pure component (ethylbenzene) and ends on a three phase (liquid-liquid-vapor) line at a critical end point.

The p-T projection of the p-T-x diagram for this system is shown schematically in Figure 3.

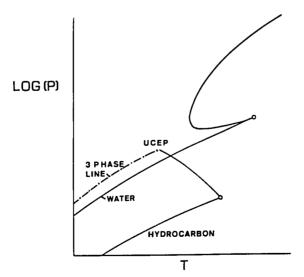


FIGURE 3. Pressure-temperature projection for ethylbenzene/water.

COMP	JNEN 15:		
(1)	Ethylbenzene;	C8H10;	[100-41-4]

(2) Water; H₂O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia. C.L. Young, Department of Physical Chemistry, University of Melbourne, Vic., Australia.

October 1986.

CRITICAL EVALUATION: (continued)

It is important to note that the three phase line on a p-T projection corresponds to three lines on the p-T-x diagram. In the region above the three phase line on the p-T projection, the pressure is greater than the vapor pressure and then a maximum of two liquid phases is possible. There may be one or two liquid phases depending on the overall composition. To the left of the critical line starting at the least volatile component it is possible to have one or two phases present depending on the overall composition.

Solubilities in the ethylbenzene + water system have been studied at elevated pressures in the publications listed in Table 6.

TABLE 6: Solubility Studies of the Ethylbenzene (1) - Water (2)

System at Elevated Pressures

Reference	p/kPa	T/K	Solubility
Guseva and Parnov (ref 9)	_a	338-507	(1) in (2)
Alwani and Schneider (ref 12) Roof (ref 13)	1.8-2.0 _b	348-387 _ ^b	critical locus $_^b$
Heidman et al. (ref 24)	0.1-10.7°	311-568	mutual

lpha Unspecified but presumably at pressures on the three phase line.

The data of Guseva and Parnov (ref 9) are thought to be unreliable. The solubilities reported by these workers are considerably larger than values obtained by other workers for the systems water + benzene, + hexane, + ethylcyclohexane and + octane. The data of Heidman $et\ al.$ (ref 24) are classified as Tentative for measurements along the three phase line. However, it should be pointed out that there is some discrepancy between the critical end point properties (574.3K, 11.2 MPa) reported by Roof (ref 13) and those reported by Heidman $et\ al.$ (568.1K, 10.68 MPa). Nevertheless, the thermodynamic functions derived from the data of Heidman $et\ al.$ are in reasonable agreement with those derived from lower temperature data (Table 3) and also with those of related hydrocarbons (e.g. benzene in water).

Alwani and Schneider (ref 12) have reported values of the critical properties along the critical curve starting at the critical point of ethylbenzene (cf. Figure 3).

b Critical point of unknown composition.

c Along three phase line.

- (1) Ethylbenzene; C_8H_{10} ; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

EVALUATOR:

G.T. Hefter, School of Mathematical and Physical Sciences, Murdoch University, Perth, W.A., Australia.

October 1986

CRITICAL EVALUATION: (continued)

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COMPONENTS: (1) Ethylbenzene; C₈H₁₀; [100-41-4] Fuhner, H. (2) Water; H₂O; [7732-18-5] Ber. Dtsch. Chem. Ges. 1924, 57, 510-5. VARIABLES: One temperature: 15°C PREPARED BY: A. Maczynski, Z. Maczynska and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 15°C was reported to be 0.014 g(1)/100 g sln.

The corresponding mole fraction, x_1 , calculated by the compilers is 2.4×10^{-5} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a stoppered volumetric cylinder, pipetted volumes or weighed amounts of (1) were added with shaking to 50, 100, or 1000 cm³ (2) until a completely clear solution was no longer obtained at the experimental temperature.

SOURCE AND PURITY OF MATERIALS:

- (1) Source not specified; commercial grade; used as received.
- (2) Not specified.

ESTIMATED ERROR:

Not specified.

- ORIGINAL MEASUREMENTS:
- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- Andrews, L.J.; Keefer, R.M.
- (2) Water; H₂O; [7732-18-5]
- J. Am. Chem. Soc. 1950, 72, 5034-7.

VARIABLES:

PREPARED BY:

One temperature: 25°C

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 0.0168 g(1)/100 g sln.

The corresponding mole fraction, x_1 , calculated by the compilers is 2.85×10^{-5} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A mixture of (1) and (2) was rotated for twenty hours in a constant temperature bath at 25°C. A sample (5-20 mL) of the aqueous phase was withdrawn and extracted with a measured volume of hexane (10-50 mL) by shaking in a glass stoppered Erlenmeyer flask. Next, the absorbance of the hexane phase was measured against a hexane blank on the Beckman spectrophotometer.

SOURCE AND PURITY OF MATERIALS:

- (1) Eastman Kodak Co. white label; fractionally distilled; b.p. 136.0°C.
- (2) Not specified.

ESTIMATED ERROR:

Not specified.

COMPONENTS: ORIGINAL MEASUREMENTS: Klevens, H.B. (1) Ethylbenzene; C₈H₁₀; [100-41-4] (2) Water; H₂O; [7732-18-5] J. Phys. Chem. 1950, 54, 283-98. VARIABLES: PREPARED BY: M.C. Haulait-Pirson Temperature: 25°C

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be $0.175 \text{ g(1)} \quad \text{L}^{-1} \text{ sln and } 0.00164 \text{ mol(1)} \quad \text{L}^{-1} \text{ sln.}$

The corresponding mass percent and mole fraction calculated by the compiler are 0.0175 g(1)/100 g sln and $x_1 = 2.9 \times 10^{-5}$.

AUXILIARY INFORMATION

The solubility of (1) in (2) was determined by shaking small amounts of (1) in 1 liter of (2) for as long (2) not specified. as three months. Aliquots were removed and concentrations determined by spectra.

METHOD/APPARATUS/PROCEDURE:

SOURCE AND PURITY OF MATERIALS:

- (1) not specified.

ESTIMATED ERROR:

not specified.

- (1) Ethylbenzene; C_8H_{10} ; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Bohon, R.L.; Claussen, W.F.

J. Am. Chem. Soc. 1951, 73, 1571-8.

VARIABLES:

PREPARED BY:

Temperature: 0.4-42.8°C

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

t/°C	g(1)/100g sln ^a (compiler)	$10^5 x_1$ (compiler)
0.4	0.0219	3.71
5.2	0.0213	3.61
20.7	0.0207	3.51
21.2	0.0207	3.51
25.0	0.0208 ^b	3.53
25.6	0.0209	3.54
30.2	0.0211	3.58
34.9	0.0221	3.75
42.8	0.0231	3.92

^a Solubilities of (1) in (2) were reported as "optical density" (absorbance) measurements. Solubilities were calculated by the compiler using the Beer-Lambert law, the stated cell path-length (1 cm) and the authors' "extinction coefficients" (absorptivities) and corrected optical densities. This gave a solubility of g(1)/L sln which was then converted to g(1)/100g sln by assuming a solution density of 1.00 kg/L.

 b Given in the original paper as 0.208g(1)/L sln.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

A round-bottomed flask containing about 4 mL of (1) and 400 mL of (2) was evacuated, suspended in a thermostat, shaken for 24h and then allowed to settle for at least another 24h. Next, desired quantities of the water layer were syphoned into 6 glass-stoppered Erlenmeyer flasks. These 6 flasks had previously been tared, partially filled with a suitable amount of diluent water, and reweighed. Weighed portions of the samples were inserted into a quartz cuvette and measured in a Beckman DU spectrophotometer. Absorbances were corrected for adsorption of (1) onto the walls of the cuvette.

SOURCE AND PURITY OF MATERIALS:

- (1) Koppers Co., purified by redistillation, several washings, and passing through silica gel. Purity was determined by refractometry (no values given).
- (2) Air-free conductivity water, no other details given.

ESTIMATED ERROR:

Temp. ± 0.02°C

Soly. ± 0.5% relative

COMPONENTS: (1) Ethylbenzene; C₈H₁₀; [100-41-4] Filippov, T.S.; Furman, A.A. (2) Water; H₂O; [7732-18-5] Zh. Prikl. Khim. 1952, 25, 895-7. VARIABLES: PREPARED BY: Temperature: 18.2-49.5°C A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of water in ethylbenzene

t/°C	g(2)/100 g sln	$10^3 x_2$ (compiler)
18.2	0.0296	1.74
18.3	0.0308	1.81
19.7	0.0327	1.92
22.3	0.0352	2.07
23.4	0.0360	2.12
24.2	0.0388	2.28
27.2	0.0494	2.91
29.8	0.0595	3.50
31.6	0.0648	3.81
32.1	0.0679	4.05
34.2	0.0745	4.38
35.1	0.0777	4.56
36.6	0.0835	4.90
38.8	0.0917	5.38
41.5	0.1005	5.90
43.1	0.1070	6.27
47.2	0.1225	7.18
49.5	0.1300	7.62

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Weighed amounts of both components were placed in glass tubes, 40 mm across and 65 mm long, and shaken. Clear and cloud points were observed 5-6 times to within 0.2-0.3°C.

SOURCE AND PURITY OF MATERIALS:

- (1) source unspecified; distilled; no turbidity if cooled to -10 or -20°C.
- (2) twice distilled.

ESTIMATED ERROR:

temp: \pm 0.3°C

soly: not specified

- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Morrison, T.J.; Billett, F.

J. Chem. Soc. 1952, 3819-22.

VARIABLES:

One temperature: 25°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25° C was reported to be 0.00155 mol(1)/1000 g(2).

The corresponding mass percent and mole fraction, x_1 , calculated by compilers are 0.0165 g(1)/100 g sln and $x_1 = 2.8 \times 10^{-5}$.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

After an excess of (1) had been shaken with about 1 dm³ of (2) for about a week, a known volume of saturated solution was made slightly alkaline, and a stream of pure air passed through to drive off the (1). After passage through a silica tube packed with cupric oxide and heated to redness, the (2) was removed by concentrated sulfuric acid and calcium chloride and the carbon dioxide absorbed and weighed in soda-asbestos. The precautions usual in organic combustions were taken.

SOURCE AND PURITY OF MATERIALS:

- (1) source not specified; purest obtainable material; distilled; purity not specified.
- (2) not specified.

ESTIMATED ERROR:

temp. ± 0.1°C

- Ethylbenzene; C_8H_{10} ; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Jones, J.R.; Monk, C.B.

J. Chem. Soc. 1963, 2633-5.

VARIABLES:

Temperature: 25-35°C

PREPARED BY:

A. Maczynski, Z. Maczynska and

A. Szafranski

EXPERIMENTAL VALUES:

Solubility of Water in Ethylbenzene

<u>t∕°C</u>	10^4 mL (2)/mL (1)
25	3.7
30	4.3
35	5.3

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a thermostatted glass stoppered flask 10-25 mL(1) was shaken for min 4 hrs. with tritiated water (a few mL of HTO equivalent to ca. 2 mci/mL) and decanted. A 5-mL aliquot was reshaken for 4 hrs. with 5 mL H₂O in a 10 mL flask, sampled and assayed with a Nuclear Enterprises type 8301 liquid scintillation counter. The two-stage process eliminates quencing effects (due to solvent) on the scintillator.

SOURCE AND PURITY OF MATERIALS:

- Laboratory grade; dried over CaCl₂ and fractionally distilled (1)
- (2) Not specified.

ESTIMATED ERROR:

Soly. ±5% to ±1% (average deviation)

- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

McAuliffe, C.

Nature (London) 1963, 200, 1092-3.

VARIABLES:

PREPARED BY:

One temperature: 25°C

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25° C was reported to be 0.0159 g(1)/100 g sln.

The corresponding mole fraction, x_1 , calculated by the compilers is 2.70×10^{-5} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solution of (1) in (2) was prepared by either shaking vigorously on a reciprocal shaker or stirring for several days with a magnetic stirrer. A 0.05 mL or 0.10 mL sample of the hydrocarbonsaturated water was injected directly into a gas liquid chromatograph.

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co.; 99+%; used as received.
- (2) Distilled.

ESTIMATED ERROR:

Temp. ±1.5°C

Soly. 0.0008 (std. dev. of mean)

COMPONENTS:	ORIGINAL MEASUREMENTS:
(1) Ethylbenzene; C ₈ H ₁₀ ; [100-41-4]	Guseva, A.N.; Parnov, E.I.
(2) Water; H ₂ O; [7732-18-5]	Zh. Fiz. Khim. 1964, 38, 805-6.
VARIABLES: Temperature: 115.0 - 233.5°C	PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

t/°C	g(1)/100 g sln	$10^4 x_1$ (compiler)
115.0	0.0513	0.871
140.5	0.119	2.02
170.5	0.355	6.04
210.0	0.661	11.27
233.5	1.129	19.33

AUXILIARY INFORMATION

AUXILIARY INFORMATION		
METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:	
The measurements were made in sealed glass tubes. No details	(1) not specified.	
were reported in the paper.	(2) not specified.	
	ESTIMATED ERROR:	
	not specified.	
	REFERENCES:	

COMPONENTS: (1) Ethylbenzene; C₈H₁₀; [100-41-4] Englin, B.A.; Plate, A.F.; Tugolukov, V.M.; Pryanishnikova, M.A. (2) Water; H₂O; [7732-18-5] Khim. Tekhnol. Topl. Masel 1965, 10, 42-6. VARIABLES: PREPARED BY: Temperature: 10-30°C A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of Water in Ethylbenzene

t/°C	g(2)/100 g sln	$10^3 x_2$ (compiler)
10	0.0275	1.62
20	0.0373	2.19
30	0.0502	2.95

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Component (1) was introduced into a thermostatted flask and saturated for 5 hr. with (2). Next, calcium hydride was added and the evolving hydrogen volume measured and hence the concentration of (2) in (1) was evaluated.

SOURCE AND PURITY OF MATERIALS:

- (1) Not specified.
- (2) Not specified.

ESTIMATED ERROR:

Not specified.

COMPONENTS: (1) Ethylbenzene; C₈H₁₀; [100-41-4] McAuliffe, C. (2) Water; H₂O; [7732-18-5] J. Phys. Chem. 1966, 70, 1267-75. VARIABLES: One temperature: 25°C PREPARED BY: A. Maczynski, Z. Maczynska, and A. Szafranski

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be $152 \text{ g(1)}/10^6 \text{ g(2)}$.

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.0152 g(1)/100 g sln and 2.57 x 10^{-5} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

In a 250-mL bottle, 10-20 mL of (1) was vigorously shaken for 1 hr, or magnetically stirred for 1 day, with 200 mL of (2) at 25°C. The bottle was set aside for 2 days to allow droplets of undissolved (1) to separate. Absence of emulsion was checked microscopically. A sample of the hydrocarbon-saturated water was withdrawn with a Hamilton syringe and gas liquid chromatographed in conjunction with a flame-ionization detector.

SOURCE AND PURITY OF MATERIALS:

- Phillips Petroleum or Columbia Chemical; used as received.
- (2) distilled.

ESTIMATED ERROR:

temp. ± 1.5°C soly. 8 g(1)/10⁶ g(2) (standard deviation of mean)

- (1) Ethylbenzene; C_8H_{10} ; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Polak, J.; Lu, B.C.-Y.

Can. J. Chem. 1973, 51, 4018-23.

VARIABLES:

PREPARED BY:

Temperature: 0-25°C

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water .

t/°C	mg(1)/kg(2)	g(1)/100 g sln (compiler)	10 ⁴ x ₁ (compiler)
0(a)	197(c)	0.0197	3.34
25 (b)	177(c)	0.0177	3.00

Solubility of water in ethylbenzene

t/°C	mg(2)/kg(1)	g(2)/100 g sln (compiler)	10 ³ x ₂ (compiler)
0(a)	178(d)	0.0178	1.05
25 (b)	442 (e)	0.0442	2.60

a-e See "Estimated Error"

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Approximately 50 mL of (1) together with (2) were placed in a 125 mL Hypo-vial which was closed with a teflon coated rubber septum and placed in a constant-temperature water bath. The system was stirred magnetically for 24 hr and left in The system was stirred the bath for 3 days or was kept in the bath without stirring for 7 days, before samples were taken for analysis. The solubility of water in the organic layer was determined by Karl Fischer titration and the

solubility of hydrocarbon in the water layer was determined by gas

chromatography.

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Co.; pure grade reagent (99+%); shaken three times with distilled water.
- (2) distilled.

ESTIMATED ERROR:

temp. (a) \pm 0.02°C, (b) \pm 0.01°C soly. (c) \pm 1.7%, (d) \pm 4.7%, (e) \pm 3.1% (from two or three determinations)

COMPONENTS: (1) Ethylbenzene: C.H.:: [100-

(1) Ethylbenzene; C₈H₁₀; [100-41-4]

(2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Brown, R.L.; Wasik, S.P.

J. Res. Natl. Bur. Stds. A. <u>1974</u>, 78, 453-60.

VARIABLES:

Temperature: 4.5-20.1°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of Ethylbenzene in Water

t/°C	$g(1)/100 \text{ g sln}^a$	$\frac{10^5 x_1 \text{ (compiler)}}{}$
4.5 6.3 7.1 9.0 11.8 12.1 15.1	0.0196 ± 0.0004 0.0192 ± 0.0004 0.0186 ± 0.0006 0.0187 ± 0.0004 0.0181 ± 0.0005 0.0183 ± 0.0004 0.0180 ± 0.0005 0.0184 ± 0.0005	3.33 3.26 3.16 3.18 3.07 3.11 3.06 3.12
20.1	0.018 ± 0.0004^{D}	3.1

^a Errors given as standard deviations.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography. The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. Basically, the hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 cm of water. The vapor was subsequently analysed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

SOURCE AND PURITY OF MATERIALS:

- (1) 99.99 mole per cent purity; source and methods of purification not specified.
- (2) Distilled.

ESTIMATED ERROR:

Temperature: ±0.01°C

Solubility: See Table above.

 $^{^{\}mathcal{O}}$ Typographical error in original publication, digit missing in fourth decimal place.

COMPONENTS: (1) Ethylbenzene; C₈H₁₀; [100-41-4] Sutton, C.; Calder, J.A. (2) Water; H₂O; [7732-18-5] J. Chem. Eng. Data 1975, 20, 320-2. VARIABLES: One temperature: 25°C PREPARED BY: A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be 161.2 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.01612 g(1)/100 g sln and 2.734×10^{-5} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:	SOURCE AND PURITY OF MATERIALS:
The concentration of (1) in (2) was determined by gas chromatography.	(1) Aldrich Chemical Co. or Matheson Coleman and Bell 99+%.
	(2) distilled.
	ECTIVATED EDDOR.
	ESTIMATED ERROR:
	temp. ± 0.1°C
	soly. 0.9 mg(1)/kg(2) (the standard deviation of the
	mean for six replicates)
	REFERENCES:
	i i

- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Price, L.C.

Am. Assoc. Petrol. Geol. Bull. 1976, 60, 213-44.

VARIABLES:

One temperature: 25°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C and at system pressure was reported to be 131.0 mg(1)/kg(2). The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.0131 g(1)/100 g sln and 2.22 x 10^{-5} .

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The solubility was determined at laboratory temperatures by use of screw-cap test tubes. The (1) phase floated on top of the water and insured saturation of the (2) phase in 2 to 4 days. Analyses were carried out by GSC using a Hewlett-Packard model 5751 gas chromatograph with dual-flame ionization detectors. Many details are given in the paper.

SOURCE AND PURITY OF MATERIALS:

- (1) Phillips Petroleum Company; Chemical Samples Company or Aldrich Chemical Company; 99+8.
- (2) distilled.

ESTIMATED ERROR:

temp. ± 1°C

 $soly. \pm 1.4 mg(1)/kg(2)$

- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Korenman, I.M.; Aref'eva, R.P.

Patent USSR, 553 524, 1977.04.05 C.A. 87:87654.

VARIABLES:

One temperature: 20°C

PREPARED BY:

A. Maczynski

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 20°C was reported to be 0.21 g(1) L^{-1} (2).

The corresponding mass percent and mole fraction, x_1 , calculated by the compiler are 0.021 g(1)/100 g sln and 3.6 x 10^{-5} . The assumption that 1 dm³ sln = 1 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

About 100-500 mL(2) was placed in a glass cylinder and 10-50 mg of an insoluble indicator was added and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall 2-3 cm above the liquid layer. After each drop of (1), the mixture was vigorously mixed for 0.5-1.5 min.

SOURCE AND PURITY OF MATERIALS:

- (1) not specified.
- (2) not specified.

ESTIMATED ERROR:

not specified.

- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Korenman, I.M.; Aref'eva, R.P.

Zh. Prikl. Khim. 1978, 51, 957-8.

VARIABLES:

Temperature: 25°C

PREPARED BY:

A. Maczynski and Z. Maczynska

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at $25^{\circ}C$ was reported to be 0.18 g(1) L^{-1} sln.

The corresponding mass percent and mole fraction, x_1 , calculated by the compilers are 0.018 g(1)/100 g sln and 3.1 x 10^{-5} . The assumption that 1.00 L⁻¹ = 1.00 kg sln was used in the calculation.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

About 200-500 mL (2) was placed in a ground-joint glass cylinder and 20-50 mg of an insoluble indicator (dithizon, phenolphthalein, etc.) was added, and (1) was microburetted until the indicator floated to form a colored thin layer on the cylinder wall above the liquid layer. Blanks were made to determine the excess of (1).

SOURCE AND PURITY OF MATERIALS:

- (1) Not specified.
- (2) Not specified.

ESTIMATED ERROR:

Soly. 0.01 g(1) L⁻¹ sln (std. dev. from 6 determinations).

- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Krzyzanowska, T.; Szeliga, J.

Nafta (Katowice), 1978, 12, 413-7.

VARIABLES:

PREPARED BY:

One temperature: 25°C

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25° C was reported to be 131.0 mg(1)/kg(2).

The corresponding mass percent and mole fraction, x_1 , calculated by compiler are 0.0131 g(1)/100 g sln and 2.22 x 10^{-5} .

Editor's Note: Based on the results for this and other hydrocarbon-water systems, uncertainity exists about whether the datum compiled here is independent of that of Price for the same system.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The saturated solutions of (1) in (2) were prepared in two ways. First, 200 µL of (1) was injected into 20 mL of (2) and thermostatted at 25°C. Second, the mixture of (1) and (2) as above was thermostatted at 70°C and then cooled to 25°C. The time required to obtain equilibrium was three weeks. The solubility of (1) in (2) was measured by glc. A Perkin-Elmer model F-11 gas chromatograph equipped with a 100-150 mesh Porasil column (70°C) and a flame ionization detector was used. Saturated solutions of heptane in (2) were used as standard solutions.

SOURCE AND PURITY OF MATERIALS:

- (1) not specified.
- (2) not specified.

ESTIMATED ERROR:

soly. 3.4 mg(1)/kg(2) (standard
deviation from 7-9 determinations).

- (1) Ethylbenzene; C_8H_{10} ; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.; Deguchi, T.; Nagai, H.

Chem. Lett. 1981, 225-8.

VARIABLES:

Temperature: 15-45°C

PREPARED BY:

M.C. Haulait-Pirson

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

t/°C	g(1)/L	g(1)/100 g sln ^a	$\frac{10^4x_1}{}^{a}$
15	0.176 ± 0.009	0.0176	2.99
25	0.181 ± 0.006	0.0182	3.09
35	0.194 ± 0.006	0.0195	3.31
45	0.215 ± 0.004	0.0217	3.69

a Assuming the solution density to be that of pure water at the same temperature (ref. 1).

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

The apparatus used for attaining solubility equilibrium is described in detail in the paper. Liquid (1) and redistilled (2) were placed in a vessel and a thermostatted funnel respectively. The solute vapor, generated by bubbling air through the liquid solute was introduced into the funnel and circulated by means of a The circulation rate was 2 L/ pump. Solubility equilibria were min. attained within 5 min. Then portions of 10 mL of the aqueous sln were transferred into funnels to which 10 $\,$ mL of chloroform had been added. Experimental procedures involved in spectrophotometric measuring the chloroform extracts were not reported REFERENCES: The solubility runs were made such that the temperature of solute reservoir was made to vary while that of solvent phase was held constant. solubility obeys Henry's law at constant solvent temperature. Solubility values were calculated from Henry's law constants.

SOURCE AND PURITY OF MATERIALS:

- (1) analytical reagent grade used as purchased.
- (2) redistilled.

ESTIMATED ERROR:

soly. : given above

1. CRC Handbook of Chemistry and Physics, R.C. Weast, Editor, CRC Press, Florida, 63rd edn, 1982, pF-11.

- (1) Ethylbenzene; $C_{8}H_{10}$; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Araki, M.;

Deguchi, T.; Nagai, H.

Bull. Chem. Soc. Jpn. 1982, 55, 1054-62.

VARIABLES:

PREPARED BY:

Temperature: 15-45°C

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water .

t /°C	10 ³ mol(1)/dm ³ sln	g(1)/100 g sln (compiler) ^a	$\frac{10^5 x_1}{(\text{compiler})^a}$
15	1.51 ± 0.08	0.0160	2.72
25	1.59 ± 0.05	0.0169	2.87
35	1.54 ± 0.05	0.0176	2.99
45	1.83 ± 0.05	0.0196	3.33

a Assuming solution densities to be the same as those of pure water at the same temperature (ref 1).

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The apparatus is similar to an earlier design (ref 2) and is described in detail in the paper. 100-200 cm³ of (2) and 10-20 cm³ of liquid (1) were placed in separate but connected thermostatted flasks. After thermal equilibrium was established a recirculating stream of air was used to vaporize liquid (1) and to transport the vapor to the flask Five 10 cm3 aliquots containing (2). were withdrawn into separatory funnels. The concentration of (1) in (2) was then determined by extraction into chloroform followed by UVspectrophotometry. Standards for the spectrophotometry were prepared by weight from pure liquid solutes.

SOURCE AND PURITY OF MATERIALS:

- (1) Analytical reagent grade (Wako Pure Chemical Ind. Ltd.), stated purity 98.0%, used without further purification.
- (2) Redistilled; no further details given.

ESTIMATED ERROR:

soly. see table, type of error not specified. temp. \pm 0.01°C.

- Kell, G.S.
 J. Chem. Eng. Data <u>1975</u>, 20, 97.
- Sanemasa, I.; Araki, M.;
 Deguchi, Y.; Nagai, H.
 Chem. Lett. 1981, 225-8.

- (1) Ethylbenzene; C_8H_{10} ; [100-41-4]
- (2) Water; H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Sanemasa, I.; Arakawa, S.; Araki, M.; Deguchi, T. Bull. Chem. Soc. Jpn. 1984, 57, 1539-44.

VARIABLES:

One Temperature: 25°C

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in water at 25°C was reported to be $1.62 \times 10^{-3} \text{ mol}(1)/\text{dm}^3 \text{ sln.}$ Assuming a solution density of 1.00 kg/dm^3 this corresponds to a solubility of $0.0172 \text{ g}(1)/100 \text{ g sln, } x_1 = 2.92 \times 10^{-5},$ calculated by the compiler.

AUXILIARY INFORMATION

METHOD /APPARATUS / PROCEDURE:

The apparatus used is described in detail in ref 1. The method involves the introduction of solute vapor(1) into liquid (2) by bubbling air through liquid (1) using a recirculating pump in a closed system. After solubility equilibrium was attained an aliquot of the saturated aqueous solution was withdrawn and analysed by solvent extraction - UV spectrophotometry.

SOURCE AND PURITY OF MATERIALS:

- Analytical reagent grade source and purity not stated, used without further purification.
- (2) Deionized and redistilled; no further details given.

ESTIMATED ERROR:

Not specified.

REFERENCES:

 Sanemasa, I., Araki, M.; Deguchi, T.; Nagai, H. Bull. Chem. Soc. Jpn. 1982, 55, 1054-62.

- (1) Ethylbenzene; C_8H_{10} ; [100-41-4]
- (2) Water, H₂O; [7732-18-5]

ORIGINAL MEASUREMENTS:

Heidman, J.L.; Tsonopoulos, C.; Brady, C.J.; Wilson, G.M.

A. I. Ch. E. J. 1985, 31, 376-84.

VARIABLES:

Temperature: 311-568 K
Pressure: 0.01-10.7 MPa

PREPARED BY:

G.T. Hefter

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in water

T/K	p /MPa	104 x1	g(1)/100 g sln (compiler)
311.5	a	0.32	0.019
311.5	_	0.32	
367.6	0.111	0.86	0.051
423.4	0.627	2.19	0.129
479.5	2.32	6.0	0.35
536.1	6.50	32.5	1.88
552.8	8.59	37.5	2.17

a Not specified.

(continued)

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Experimental procedure was similar to that used in ref. 1. Hydrocarbons were determined by gas chromatography and water by Karl Fischer titration. Critical points were determined by the synthetic method using visual observation. This aspect of the procedure is discussed in detail in the paper.

SOURCE AND PURITY OF MATERIALS:

- (1) Aldrich 99+ mol %; water free purity ≥ 99.9 mol %, checked by gas chromatography.
- (2) Distilled; no details given.

ESTIMATED ERROR:

soly. ± 5%, relative precision of replicate analyses. temp. not stated.

press. ± 1%; type of error not stated.

REFERENCES:

 Tsonopoulos, C.; Wilson, G.M. A. I. Ch. E. J. 1983, 29, 990-9.

- (1) Ethylbenzene; $C_{8}H_{10}$; [100-41-4]
- (2) Water, H₂O; [7732-18-5]

(continued)

Solubility of water in ethylbenzene

<i>T</i> /K	<i>p</i> /MPa	102 x2	g(2)/100 g sln (compiler)
310.9	0.0091 ^a	0.43	0.073
367.6	0.111	1.86	0.320
423.4	0.627	5.96	1.06
479.5	2.32	16.3	3.20
536.1	6.50	40.8	10.5
550.4	8.27	47.2	13.2
568.1 ^b	10.68 ^b	69.1 ^b	27.5

- a Estimated by the authors from pure component data.
- b Three phase critical point.

The three phase critical point was reported to be 568.1 \pm 0.6 K, 10.68 \pm 0.04 MPa and x_1 = 5.83 x 10⁻³ (3.34 g(1)/100 g sln, compiler).

The authors also report an equation providing a fit of their own and literature data over the range 273-568 K, viz.

$$\ln x_1 = -185.1695 + 7348.55/T + 26.34525 \ln T$$

$$\ln x_2 = -0.37215 - 4.4626 (T_r^{-1} - 1) - 0.38596 (1 - T_r)^{1/3}$$

$$- 2.59850 (1 - T_r)$$

where $T_n = T/568.1$

- (1) Ethylbenzene; $C_{8}H_{10}$; [100-41-4]
- (2) Artificial seawater

ORIGINAL MEASUREMENTS:

Brown, R.L.; Wasik, S.P.

J. Res. Natl. Bur. Stds. A. <u>1974</u>, 78, 453-60.

VARIABLES:

Temperature: 0-20°C

Salinity: 34.42 g salts/kg sln

PREPARED BY:

G.T. Hefter and D.G. Shaw

EXPERIMENTAL VALUES:

Solubility of ethylbenzene in artificial seawater

t/°C	$g(1)/100 \text{ g sln}^a$	$\frac{10^5 x_1}{10^5 x_1}$ (compiler)
0.19	0.0140 (0.0002)	2.44
5.32	0.0133 (0.0003)	2.31
10.05	0.0129 (0.0003)	2.25
14.96	0.0125 (0.0003)	2.18
20.04	0.0122 (0.0003)	2.12

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

Solubilities were calculated from partition coefficient measurements for the hydrocarbon between an aqueous solution and its vapor using headspace chromatography.

The apparatus and the method of obtaining the partition coefficients are described in detail in the paper. The hydrocarbon was introduced as a vapor (to avoid emulsification) into a glass equilibration cell containing about 45 L of water. The vapor was subsequently analysed by gas chromatography using He as the carrier. Possible sources of error are discussed in detail although the source of vapor pressure data used to calculate solubilities are not given.

SOURCE AND PURITY OF MATERIALS:

- (1) 99.99 mole per cent purity; source and methods of purification not specified.
- (2) Prepared according to ref 1. Purity not specified.

ESTIMATED ERROR:

Temperature: ±0.01 K

Solubility: see Table above

REFERENCES:

 Sverdrup, H.U.; Johnson, M.W.; Fleming, R.H.; The Oceans, 1942, Prentice-Hall, Englewood Cliffs, New Jersey, p186.

- (1) Ethylbenzene; C₈H₁₀; [100-41-4]
- (2) Artificial seawater (ref 1)

ORIGINAL MEASUREMENTS:

Sutton, C.; Calder, J.A.

J. Chem. Eng. Data 1975, 20, 320-2.

VARIABLES:

One temperature: 25.0°C

One salinity: 34.5 g salts/kg sln

PREPARED BY:

M. Kleinschmidt

EXPERIMENTAL VALUES:

The solubility of ethylbenzene in artificial seawater is reported to be 111.0 mg (1)/kg sln. The corresponding mass percent and mole fraction, x_1 calculated by the compiler are 0.01110 g(1)/100 g sln and 1.9 x 10^{-5} assuming the artificial seawater composition of ref 1.

AUXILIARY INFORMATION

METHOD/APPARATUS/PROCEDURE:

A test tube containing (1) was placed in a flask containing (2) thus allowing for equilibration through the vapor phase. The saturated solution was extracted with hexane and analyzed by gas chromatography.

SOURCE AND PURITY OF MATERIALS:

- (1) from either Aldrich Chemical Co. or Matheson Coleman and Bell, 99+% pure.
- (2) made from doubly distilled water and salts 99+% pure.

ESTIMATED ERROR:

temp. ± 0.1°C

soly. 1.3 (std. dev.)

REFERENCES:

Lyman, J.; Fleming, R.H.;
 J. Mar. Res. <u>1940</u>, 3, 135.